

## LA-UR-19-21784

Approved for public release; distribution is unlimited.

Title: Integrating CryoEM and Molecular dynamic simulations

Author(s): Lopez Bautista, Cesar Augusto  
Gnanakaran, Sandrasegaram

Intended for: IC report

Issued: 2019-02-28

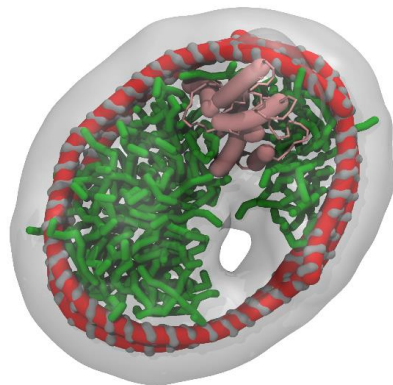
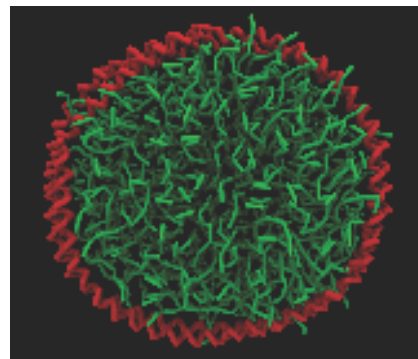
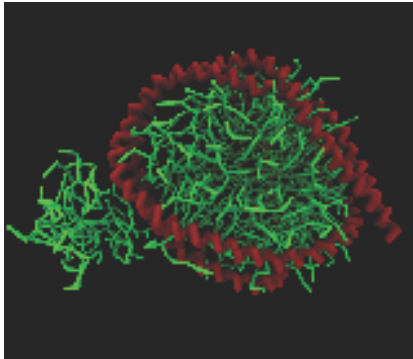
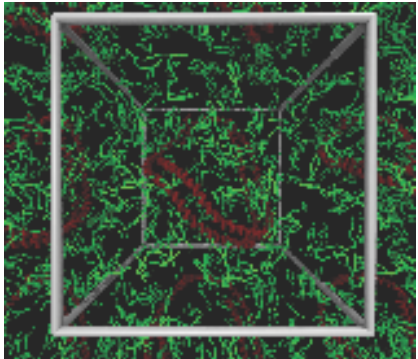
---

**Disclaimer:**

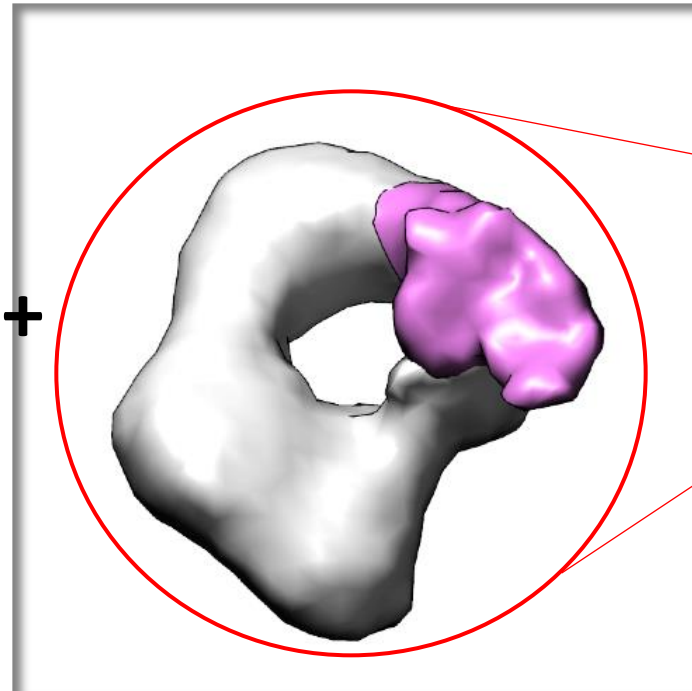
Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

# Integrating CryoEM and Molecular dynamic simulations

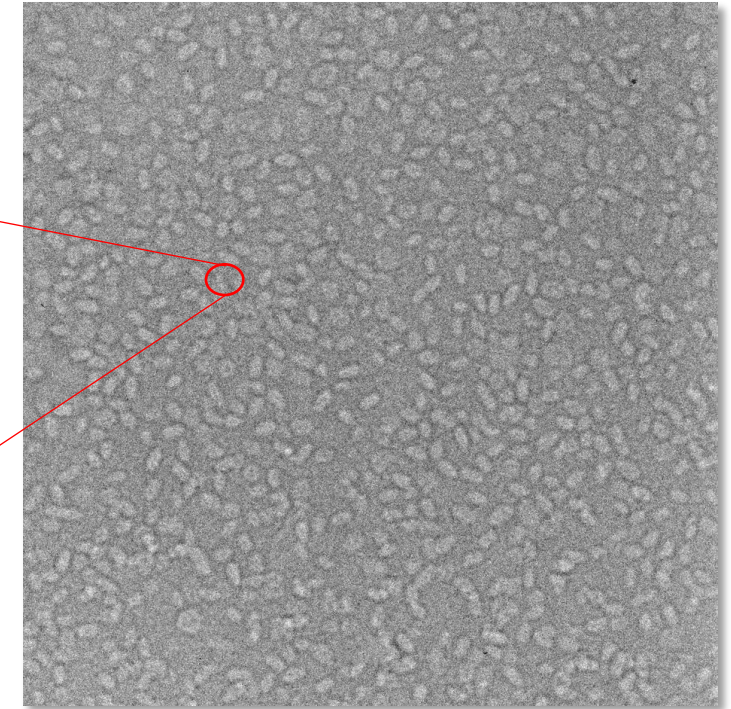
Computational nanodisc self-assembly



CryoEM MD-assisted reconstruction



Experimental validation



López et al. analyze the structure and dynamics of lipid nanodiscs, both empty and in complex with pro-apoptotic BAX protein. Information from the computational-derived structures prompted changes in image processing strategy, which led to quality improvements in Cryo-EM reconstructions. Together, these findings provide novel insights on the activity of BAX.